

# Argonne National Laboratory

HARTREE-FOCK WAVE FUNCTIONS  
AND COMPUTED ONE-ELECTRON PROPERTIES  
FOR OXYGEN MONOFLUORIDE ( $OF, ^2\Pi$ )  
AT SIX INTERNUCLEAR SEPARATIONS

by

P. A. G. O'Hare and Arnold C. Wahl

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June 1970



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A recent paper<sup>1</sup> by the present author describes a self-consistent-field calculation of the OF system. Self-consistent-field calculations were carried out at six internuclear separations including the equilibrium separation obtained via a minimum search of the potential energy of space-charge distributions, the complete wave function was determined at each internuclear separation. The present paper gives details concerning the effect of the six internuclear separations, respectively, on the electronic properties.

### II. COMPUTATIONAL PROCEDURE, COMPUTED WAVE FUNCTIONS, AND ONE-ELECTRON PROPERTIES

Self-consistent-field wave functions for the oxygen molecule were calculated by Hartree's successive iteration method.<sup>2</sup> "Stoer," has been chosen to describe the numerical integration of the wave function and its derivative. The wave functions and derivatives are obtained by the addition of two terms, the first term being 1.44207 and the second term, the electron density, is given by the following equation:

$$\rho = \frac{1}{4\pi} \int \frac{1}{r^2} dr$$

The equilibrium internuclear separation was determined numerically. An example of the iterative procedure for determining the equilibrium internuclear separation is given below.

<sup>1</sup> 1 bohr = 0.02417 Å.



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ABSTRACT

The Roothaan expansion method has been used to compute self-consistent-field wave functions close to the Hartree-Fock limit for oxygen monofluoride (OF) at six internuclear separations. A Dunham analysis yielded 2.4958 bohrs for  $r_e$ ; the corresponding energy was -174.19502 Hartrees. The detailed wave functions are given together with the corresponding computed energies and one-electron properties. At  $r_e$ , the dipole moment was found to be 0.36 D with the negative end of the dipole at the fluorine atom.

I. INTRODUCTION

A recent paper<sup>1</sup> by the present authors described a Hartree-Fock investigation of the OF system. Self-consistent-field wave functions were computed at six internuclear separations including the equilibrium bond length ( $r_e$ ) obtained via a Dunham analysis of the potential energy curve. Because of space limitations, the complete wave functions were not included in the journal article.<sup>1</sup> The present report gives detailed wave functions for each of the six internuclear separations, together with the corresponding one-electron properties.

II. COMPUTATIONAL PROCEDURE, CALCULATED WAVE FUNCTIONS, AND ONE-ELECTRON PROPERTIES

Self-consistent-field wave functions for OF near the Hartree-Fock limit were calculated by Roothaan's expansion method.<sup>2</sup> The computer system, "BISON," has been described in detail by Wahl and co-workers.<sup>3</sup> Calculations were performed on an IBM-360/75 machine. The Gilbert-Bagus<sup>4</sup> accurate basis function sets were used for O( $^3P$ ) and F( $^2P$ ). Each basis set was augmented by the addition of 3d polarization functions: for O, 2.86 and 1.11,<sup>5</sup> and for F, 2.44269.<sup>6</sup> By analogy with OC<sub>1</sub>,<sup>7</sup> OF was assumed to have a  $^2\Pi_i$  ground state; the electronic structure, following Mulliken's nomenclature,<sup>8</sup> is as follows:

$$KK(z\sigma)^2(y\sigma)^2(x\sigma)^2(w\pi)^4(v\pi)^3, ^2\Pi_i. \quad (1)$$

The equilibrium internuclear separation,  $r_e$ , has not been measured experimentally. An exploratory series of calculations with minimal basis sets<sup>9</sup> for O and F gave a preliminary value of 2.52 bohrs\* (1.33 Å) for  $r_e$ (OF).

\*1 bohr = 0.52917 Å.



Accurate wave functions were then computed at internuclear separations of 2.3, 2.4, 2.5, 2.6, and 2.7 bohrs; a Dunham analysis of the results showed that the energy minimum was located at 2.4958 bohrs. An additional wave function for  $r_e = 2.4958$  bohrs was then computed. The wave functions are given in Tables I-VI. Based on previous experience,<sup>10</sup> the expansion error is estimated to be not more than 0.005 h.\*

Table VII lists the values for the total ( $E$ ), potential ( $V$ ), and kinetic ( $T$ ) energies, and the virial ( $V/T$ ). Table VIII summarizes the computed one-electron properties.

A complete discussion of the investigation on the OF system appears in Ref. 1.

TABLE I. Hartree-Fock-Roothaan Wave Function for OF at 2.3 bohrs

N	L	M	ZETA	1 $\sigma$	2 $\sigma$	3 $\sigma$	4 $\sigma$	5 $\sigma$
1	0	0	12.41800	0.0	-0.09362	-0.00032	-0.00243	-0.00304
1	0	0	6.99500	0.00003	-0.94523	0.12416	0.22233	0.08879
3	0	0	8.68100	0.00002	0.04130	0.02286	0.02743	-0.00758
2	0	0	2.92200	-0.00013	-0.00315	-0.27926	-0.47236	-0.12082
2	0	0	1.81800	0.00066	0.00085	-0.10741	-0.41165	-0.39535
2	1	0	8.45000	0.00002	-0.00079	-0.00206	0.00029	0.00701
2	1	0	3.74400	-0.00012	-0.00209	-0.03848	0.01817	0.14224
2	1	0	2.12100	0.00041	0.00181	-0.13164	-0.00186	0.34316
2	1	0	1.31800	0.00025	-0.00042	0.03172	0.03421	0.09512
3	2	0	2.86000	0.00016	0.00024	-0.02395	-0.00052	0.03351
3	2	0	1.11000	0.00009	0.00006	0.00263	0.00445	0.01335
1	0	0	-14.20100	0.08418	0.0	-0.00362	0.00320	-0.00153
1	0	0	-7.93800	0.95495	0.00010	0.23047	-0.14798	0.03357
3	0	0	-9.96200	-0.04240	-0.00004	0.02568	-0.01101	-0.00244
2	0	0	-3.33200	0.00381	0.00015	-0.46242	0.29441	-0.05485
2	0	0	-2.05700	-0.00111	-0.00065	-0.40059	0.35326	-0.12589
2	1	0	-9.43500	0.00058	-0.00002	-0.00332	-0.00407	0.00900
2	1	0	-4.24900	0.00134	0.00004	-0.02425	-0.07920	0.16490
2	1	0	-2.35600	-0.00098	-0.00036	-0.12296	-0.17450	0.36407
2	1	0	-1.43400	0.00001	-0.00028	-0.00554	-0.05231	0.20491
3	2	0	-2.44269	-0.00031	-0.00021	-0.02701	-0.02447	0.04416

ORBITAL ENERGIES                    -26.3939    -20.7113    -1.8071    -1.2309    -0.7764

N	L	M	ZETA	1 $\pi$	2 $\pi$
2	1	1	8.45000	-0.00401	-0.01054
2	1	1	3.74400	-0.04639	-0.24326
2	1	1	2.12100	-0.17047	-0.47153
2	1	1	1.31800	0.00229	-0.36651
3	2	1	2.86000	-0.02380	-0.00906
3	2	1	1.11000	-0.00135	0.00822
2	1	1	-9.43500	-0.01091	0.00279
2	1	1	-4.24900	-0.24346	0.10839
2	1	1	-2.35600	-0.47121	0.13342
2	1	1	-1.43400	-0.30150	0.20911
3	2	1	-2.44269	-0.02962	-0.01586

ORBITAL ENERGIES                    -0.7911    -0.5723

\*1 Hartree (h) = 27.20974 eV = 627.48 kcal mol<sup>-1</sup>.

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10000.0-	09000.0-	02000.0-	03000.0-	80000.0	00048.7	0	0	0
10000.0-	01000.0-	04000.0-	00000.0-	80000.0	00048.8	0	0	0
10000.0-	06000.0-	00000.0-	08000.0-	80000.0	00048.9	0	0	0
10000.0-	08000.0-	03000.0-	05000.0-	80000.0	00049.0	0	0	0
10000.0-	00000.0-	06000.0-	02000.0-	80000.0	00049.1	0	0	0
10000.0-	02000.0-	08000.0-	04000.0-	80000.0	00049.2	0	0	0
10000.0-	05000.0-	03000.0-	01000.0-	80000.0	00049.3	0	0	0
10000.0-	07000.0-	00000.0-	06000.0-	80000.0	00049.4	0	0	0
10000.0-	09000.0-	02000.0-	03000.0-	80000.0	00049.5	0	0	0
10000.0-	01000.0-	04000.0-	00000.0-	80000.0	00049.6	0	0	0
10000.0-	06000.0-	00000.0-	08000.0-	80000.0	00049.7	0	0	0
10000.0-	08000.0-	03000.0-	05000.0-	80000.0	00049.8	0	0	0
10000.0-	00000.0-	06000.0-	02000.0-	80000.0	00049.9	0	0	0
10000.0-	02000.0-	08000.0-	04000.0-	80000.0	00050.0	0	0	0
10000.0-	05000.0-	03000.0-	01000.0-	80000.0	00050.1	0	0	0
10000.0-	07000.0-	00000.0-	06000.0-	80000.0	00050.2	0	0	0
10000.0-	09000.0-	02000.0-	03000.0-	80000.0	00050.3	0	0	0
10000.0-	01000.0-	04000.0-	00000.0-	80000.0	00050.4	0	0	0
10000.0-	06000.0-	00000.0-	08000.0-	80000				

TABLE II. Hartree-Fock-Roothaan Wave Function for OF at 2.4 bohrs

N	L	M	ZETA	1σ	2σ	3σ	4σ	5σ
1	0	0	12.41800	0.0	-0.09360	-0.00036	0.00258	-0.00290
1	0	0	6.99500	0.00003	-0.94534	0.11838	-0.22977	0.08108
3	0	0	8.68100	0.00002	0.04136	0.02109	-0.02801	-0.00700
2	0	0	2.92200	-0.00013	-0.00300	-0.26513	0.48809	-0.11175
2	0	0	1.81800	0.00057	0.00071	-0.11825	0.42766	-0.35525
2	1	0	8.45000	0.00002	-0.00075	-0.00216	-0.00026	0.00741
2	1	0	3.74400	-0.00012	-0.00189	-0.03137	-0.01875	0.13559
2	1	0	2.12100	0.00038	0.00165	-0.12135	-0.00074	0.34347
2	1	0	1.31800	0.00021	-0.00040	0.02552	-0.03159	0.10413
3	2	0	2.86000	0.00015	0.00027	-0.02129	0.00008	0.03194
3	2	0	1.11000	0.00008	0.00004	0.00121	-0.00402	0.01342
1	0	0	-14.20100	0.08417	0.0	-0.00381	-0.00308	-0.00150
1	0	0	-7.93800	0.95501	0.00008	0.23454	0.14230	0.03504
3	0	0	-9.96200	-0.04242	-0.00004	0.02549	0.01075	-0.00189
2	0	0	-3.33200	0.00367	0.00015	-0.47024	-0.28332	-0.06026
2	0	0	-2.05700	-0.00094	-0.00055	-0.41526	-0.33353	-0.12723
2	1	0	-9.43500	0.00056	-0.00002	-0.00303	0.00367	0.00914
2	1	0	-4.24900	0.00119	0.00005	-0.01894	0.06890	0.16757
2	1	0	-2.35600	-0.00085	-0.00032	-0.10689	0.15478	0.36513
2	1	0	-1.43400	0.0	-0.00026	-0.00665	0.04598	0.21600
3	2	0	-2.44269	-0.00031	-0.00020	-0.02348	0.02191	0.04258

ORBITAL ENERGIES -26.3888 -20.7247 -1.7628 -1.2428 -0.7583

N	L	M	ZETA	1π	2π
2	1	1	8.45000	-0.00354	-0.01069
2	1	1	3.74400	-0.04011	-0.24461
2	1	1	2.12100	-0.14698	-0.48200
2	1	1	1.31800	-0.00206	-0.35395
3	2	1	2.86000	-0.02065	-0.00878
3	2	1	1.11000	-0.00395	0.00737
2	1	1	-9.43500	-0.01087	0.00243
2	1	1	-4.24900	-0.24777	0.09749
2	1	1	-2.35600	-0.47187	0.11907
2	1	1	-1.43400	-0.31020	0.18436
3	2	1	-2.44269	-0.02624	-0.01437

ORBITAL ENERGIES -0.7692 -0.5930



TABLE III. Hartree-Fock-Roothaan Wave Function for OF at 2.4958 bohrs

N	L	M	ZETA	1σ	2σ	3σ	4σ	5σ
1	0	0	12.41800	0.0	-0.09358	-0.00043	-0.00271	0.00271
1	0	0	6.99500	0.00002	-0.94543	0.11257	0.23630	-0.07402
3	0	0	8.68100	0.00002	0.04141	0.01930	0.02853	0.00619
2	0	0	2.92200	-0.00014	-0.00286	-0.25035	-0.50194	0.10462
2	0	0	1.81800	0.00050	0.00058	-0.12597	-0.44051	0.31705
2	1	0	8.45000	0.00002	-0.00071	-0.00218	0.00023	-0.00770
2	1	0	3.74400	-0.00012	-0.00171	-0.02566	0.01855	-0.13033
2	1	0	2.12100	0.00034	0.00150	-0.11028	0.00271	-0.34091
2	1	0	1.31800	0.00018	-0.00039	0.01947	0.02876	-0.11406
3	2	0	2.86000	0.00013	0.00028	-0.01883	0.00020	-0.03029
3	2	0	1.11000	0.00007	0.00002	-0.00008	0.00353	-0.01366
1	0	0	-14.20100	0.08416	0.0	-0.00400	0.00295	0.00144
1	0	0	-7.93800	0.95506	0.00007	0.23880	-0.13610	-0.03552
3	0	0	-9.96200	-0.04243	-0.00003	0.02537	-0.01042	0.00137
2	0	0	-3.33200	0.00355	0.00014	-0.47845	0.27115	0.06366
2	0	0	-2.05700	-0.00080	-0.00045	-0.42901	0.31374	0.12578
2	1	0	-9.43500	0.00053	-0.00002	-0.00272	-0.00331	-0.00919
2	1	0	-4.24900	0.00106	0.00005	-0.01454	-0.05995	-0.16985
2	1	0	-2.35600	-0.00074	-0.00029	-0.09175	-0.13734	-0.36364
2	1	0	-1.43400	0.0	-0.00023	-0.00746	-0.04050	-0.22681
3	2	0	-2.44269	-0.00031	-0.00019	-0.02028	-0.01963	-0.04081

ORBITAL ENERGIES -26.3845 -20.7366 -1.7264 -1.2539 -0.7408

N	L	M	ZETA	1π	2π
2	1	1	8.45000	-0.00308	-0.01080
2	1	1	3.74400	-0.03477	-0.24580
2	1	1	2.12100	-0.12574	-0.49019
2	1	1	1.31800	-0.00560	-0.34393
3	2	1	2.86000	-0.01781	-0.00829
3	2	1	1.11000	-0.00599	0.00665
2	1	1	-9.43500	-0.01081	0.00212
2	1	1	-4.24900	-0.25159	0.08734
2	1	1	-2.35600	-0.47191	0.10601
2	1	1	-1.43400	-0.31742	0.16224
3	2	1	-2.44269	-0.02317	-0.01298

ORBITAL ENERGIES -0.7515 -0.6101



TABLE IV. Hartree-Fock-Roothaan Wave Function for OF at 2.5 bohrs

N	L	M	ZETA	1σ	2σ	3σ	4σ	5σ
1	0	0	12.41800	0.0	-0.09358	-0.00043	-0.00271	0.00271
1	0	0	6.99500	0.00002	-0.94543	0.11257	0.23630	-0.07402
3	0	0	8.68100	0.00002	0.04141	0.01930	0.02853	0.00619
2	0	0	2.92200	-0.00014	-0.00286	-0.25035	-0.50194	0.10462
2	0	0	1.81800	0.00050	0.00058	-0.12597	-0.44051	0.31705
2	1	0	8.45000	0.00002	-0.00071	-0.00218	0.00023	-0.00770
2	1	0	3.74400	-0.00012	-0.00171	-0.02566	0.01855	-0.13033
2	1	0	2.12100	0.00034	0.00150	-0.11028	0.00271	-0.34091
2	1	0	1.31800	0.00018	-0.00039	0.01947	0.02876	-0.11406
3	2	0	2.86000	0.00013	0.00028	-0.01883	0.00020	-0.03029
3	2	0	1.11000	0.00007	0.00002	-0.00008	0.00353	-0.01366
1	0	0	-14.20100	0.08416	0.0	-0.00400	0.00295	0.00144
1	0	0	-7.93800	0.95506	0.00007	0.23880	-0.13610	-0.03552
3	0	0	-9.96200	-0.04243	-0.00003	0.02537	-0.01042	0.00137
2	0	0	-3.33200	0.00355	0.00014	-0.47845	0.27115	0.06366
2	0	0	-2.05700	-0.00080	-0.00045	-0.42901	0.31374	0.12578
2	1	0	-9.43500	0.00053	-0.00002	-0.00272	-0.00331	-0.00919
2	1	0	-4.24900	0.00106	0.00005	-0.01454	-0.05995	-0.16985
2	1	0	-2.35600	-0.00074	-0.00029	-0.09175	-0.13734	-0.36364
2	1	0	-1.43400	0.0	-0.00023	-0.00746	-0.04050	-0.22681
3	2	0	-2.44269	-0.00031	-0.00019	-0.02028	-0.01963	-0.04081

ORBITAL ENERGIES -26.3844 -20.7371 -1.7250 -1.2544 -0.7400

N	L	M	ZETA	1π	2π
2	1	1	8.45000	-0.00308	-0.01080
2	1	1	3.74400	-0.03477	-0.24580
2	1	1	2.12100	-0.12574	-0.49019
2	1	1	1.31800	-0.00560	-0.34393
3	2	1	2.86000	-0.01781	-0.00829
3	2	1	1.11000	-0.00599	0.00665
2	1	1	-9.43500	-0.01081	0.00212
2	1	1	-4.24900	-0.25159	0.08734
2	1	1	-2.35600	-0.47191	0.10601
2	1	1	-1.43400	-0.31742	0.16224
3	2	1	-2.44269	-0.02317	-0.01298

ORBITAL ENERGIES -0.7508 -0.6108



TABLE V. Hartree-Fock-Roothaan Wave Function for OF at 2.6 bohrs

N	L	M	ZETA	1σ	2σ	3σ	4σ	5σ
1	0	0	12.41800	0.0	-0.09356	-0.00050	0.00283	0.00249
1	0	0	6.99500	0.00002	-0.94550	0.10667	-0.24205	-0.06758
3	0	0	8.68100	0.00002	0.04144	0.01752	-0.02901	0.00522
2	0	0	2.92200	-0.00014	-0.00275	-0.23517	0.51420	0.09904
2	0	0	1.81800	0.00044	0.00047	-0.13070	0.45094	0.28182
2	1	0	8.45000	0.00003	-0.00067	-0.00213	-0.00022	-0.00788
2	1	0	3.74400	-0.00011	-0.00154	-0.02114	-0.01785	-0.12634
2	1	0	2.12100	0.00030	0.00136	-0.09893	-0.00427	-0.33588
2	1	0	1.31800	0.00017	-0.00037	0.01378	-0.02588	-0.12530
3	2	0	2.86000	0.00012	0.00030	-0.01656	-0.00039	-0.02860
3	2	0	1.11000	0.00007	0.00001	-0.00122	-0.00303	-0.01401
1	0	0	-14.20100	0.08415	0.0	-0.00419	-0.00280	0.00136
1	0	0	-7.93800	0.95510	0.00006	0.24309	0.12944	-0.03525
3	0	0	-9.96200	-0.04244	-0.00003	0.02531	0.01004	0.00089
2	0	0	-3.33200	0.00345	0.00012	-0.48679	-0.25804	0.06547
2	0	0	-2.05700	-0.00068	-0.00037	-0.44178	-0.29398	0.12235
2	1	0	-9.43500	0.00051	-0.00002	-0.00240	0.00299	-0.00915
2	1	0	-4.24900	0.00095	0.00005	-0.01094	0.05220	-0.17191
2	1	0	-2.35600	-0.00065	-0.00025	-0.07779	0.12195	-0.36028
2	1	0	-1.43400	0.0	-0.00021	-0.00795	0.03578	-0.23729
3	2	0	-2.44269	-0.00031	-0.00017	-0.01739	0.01759	-0.03891

ORBITAL ENERGIES -26.3806 -20.7486 -1.6927 -1.2654 -0.7217

N	L	M	ZETA	1π	2π
2	1	1	8.45000	-0.00266	-0.01087
2	1	1	3.74400	-0.03024	-0.24684
2	1	1	2.12100	-0.10687	-0.49663
2	1	1	1.31800	-0.00840	-0.33582
3	2	1	2.86000	-0.01528	-0.00768
3	2	1	1.11000	-0.00753	0.00607
2	1	1	-9.43500	-0.01073	0.00185
2	1	1	-4.24900	-0.25491	0.07801
2	1	1	-2.35600	-0.47153	0.09430
2	1	1	-1.43400	-0.32340	0.14257
3	2	1	-2.44269	-0.02040	-0.01168

ORBITAL ENERGIES -0.7354 -0.6260



TABLE VI. Hartree-Fock-Roothaan Wave Function for OF at 2.7 bohrs

N	L	M	ZETA	1σ	2σ	3σ	4σ	5σ
1	0	0	12.41800	0.0	-0.09355	-0.00057	-0.00294	0.00225
1	0	0	6.99500	0.00001	-0.94555	0.10065	0.24712	-0.06172
3	0	0	8.68100	0.00003	0.04147	0.01581	0.02945	0.00416
2	0	0	2.92200	-0.00015	-0.00265	-0.21980	-0.52511	0.09463
2	0	0	1.81800	0.00040	0.00038	-0.13268	-0.45953	0.24957
2	1	0	8.45000	0.00002	-0.00064	-0.00203	0.00021	-0.00796
2	1	0	3.74400	-0.00011	-0.00139	-0.01762	0.01685	-0.12346
2	1	0	2.12100	0.00027	0.00124	-0.08772	0.00559	-0.32882
2	1	0	1.31800	0.00015	-0.00036	0.00858	0.02305	-0.13747
3	2	0	2.86000	0.00011	0.00030	-0.01449	0.00053	-0.02687
3	2	0	1.11000	0.00006	0.0	-0.00220	0.00253	-0.01443
1	0	0	-14.20100	0.08415	0.0	-0.00436	0.00265	0.00127
1	0	0	-7.93800	0.95513	0.00005	0.24731	-0.12241	-0.03446
3	0	0	-9.96200	-0.04245	-0.00003	0.02531	-0.00960	0.00046
2	0	0	-3.33200	0.00336	0.00011	-0.49507	0.24417	0.06605
2	0	0	-2.05700	-0.00059	-0.00030	-0.45351	0.27436	0.11754
2	1	0	-9.43500	0.00048	-0.00002	-0.00209	-0.00270	-0.00905
2	1	0	-4.24900	0.00085	0.00004	-0.00801	-0.04550	-0.17386
2	1	0	-2.35600	-0.00057	-0.00021	-0.06517	-0.10837	-0.35563
2	1	0	-1.43400	-0.00001	-0.00018	-0.00815	-0.03169	-0.24738
3	2	0	-2.44269	-0.00030	-0.00016	-0.01480	-0.01577	-0.03693

ORBITAL ENERGIES -26.3773 -20.7591 -1.6654 -1.2757 -0.7038

N	L	M	ZETA	1π	2π
2	1	1	8.45000	-0.00228	-0.01091
2	1	1	3.74400	-0.02642	-0.24776
2	1	1	2.12100	-0.09039	-0.50177
2	1	1	1.31800	-0.01057	-0.32911
3	2	1	2.86000	-0.01305	-0.00699
3	2	1	1.11000	-0.00865	0.00563
2	1	1	-9.43500	-0.01065	0.00162
2	1	1	-4.24900	-0.25775	0.06954
2	1	1	-2.35600	-0.47085	0.08391
2	1	1	-1.43400	-0.32833	0.12517
3	2	1	-2.44269	-0.01794	-0.01047

ORBITAL ENERGIES -0.7225 -0.6390



TABLE VII. Computed Energy Results (h)

<i>R</i>	<i>E</i>	<i>V</i>	<i>T</i>	<i>-V/T</i>
2.30	-174.18344	-348.70566	174.52222	1.99806
2.40	-174.19254	-348.54726	174.35472	1.99907
2.4958	-174.19502	-348.41715	174.22213	1.99984
2.50	-174.19502	-348.41184	174.21683	1.99987
2.60	-174.19265	-348.29514	174.10249	2.00052
2.70	-174.18677	-348.19392	174.00715	2.00103

TABLE VIII. Expectation Values of Selected Operators<sup>a</sup> for OF(<sup>2</sup>Π)

<i>R</i> , bohr	2.3	2.4	2.5	2.6	2.7	2.4958
(sin <sup>2</sup> <i>A</i> )/ <i>R<sub>A</sub></i> , bohr <sup>-1</sup>	15.494	15.440	15.393	15.351	15.315	15.394
(cos <sup>2</sup> <i>A</i> )/ <i>R<sub>A</sub></i> , bohr <sup>-1</sup>	10.629	10.509	10.396	10.289	10.187	10.400
3 <i>Z<sub>A</sub><sup>2</sup></i> - <i>R<sub>A</sub><sup>2</sup></i> , bohr <sup>2</sup>	95.524	104.114	113.076	122.414	132.125	112.693
1/ <i>R<sub>A</sub></i> , bohr <sup>-1</sup>	26.123	25.949	25.788	25.640	25.502	25.794
<i>R<sub>A</sub><sup>2</sup></i> , bohr <sup>2</sup>	69.131	73.575	78.193	82.986	87.954	77.996
<i>Z<sub>A</sub><sup>2</sup></i> , bohr <sup>2</sup>	54.885	59.229	63.756	68.467	73.360	63.563
(sin <sup>2</sup> <i>B</i> )/ <i>R<sub>B</sub></i> , bohr <sup>-1</sup>	18.452	18.418	18.388	18.360	18.335	18.389
(cos <sup>2</sup> <i>B</i> )/ <i>R<sub>B</sub></i> , bohr <sup>-1</sup>	11.525	11.420	11.322	11.231	11.145	11.326
3 <i>Z<sub>B</sub><sup>2</sup></i> - <i>R<sub>B</sub><sup>2</sup></i> , bohr <sup>2</sup>	84.964	91.885	99.127	106.690	114.577	98.816
1/ <i>R<sub>B</sub></i> , bohr <sup>-1</sup>	29.977	29.838	29.710	29.591	29.481	29.715
<i>R<sub>B</sub><sup>2</sup></i> , bohr <sup>2</sup>	63.851	67.461	71.218	75.125	79.180	71.058
<i>Z<sub>B</sub><sup>2</sup></i> , bohr <sup>2</sup>	49.605	53.115	56.782	60.605	64.586	56.625
<i>ζ</i>	25.070	24.691	24.343	24.024	23.731	24.357
<i>η</i>	0.884	0.921	0.955	0.986	1.014	0.954
<i>X<sup>2</sup></i> , bohr <sup>2</sup>	14.246	14.345	14.436	14.520	14.594	14.433
<i>Z</i> , bohr	1.148	1.274	1.395	1.512	1.625	1.390

<sup>a</sup>Center *A* = O, *B* = F.

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